Idoxuridine

Idoxarianic						
54-42-2	DTXSID2	04523				

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 1.31

Global applicability domain: Inside

Local applicability domain index: 3.49e-01

Confidence level: 7.44e-01

Nearest Neighbors from the Training Set

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Tris(2-hydroxyethyl) isocyanurate

Measured: 1.58 Predicted: 1.61

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Triisopropanolamine

Measured: 5.75e-01 Predicted: 7.42e-01

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Hexamethylphosphoramide

Measured: 5.01e-01 Predicted: 7.23e-01

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Triethanolamine Measured: 3.89 Predicted: 2.97

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Cycloheximide Measured: 2.82 Predicted: 2.70